

Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security An Initiative

The objective of this ten-year vision, which is in line with the Department of Energy's Strategic Goals for Scientific Discovery and Innovation, is to focus the computational science experiences gained over the past ten years on the opportunities introduced with exascale computing to revolutionize our approaches to energy, environmental sustainability and security global challenges.

Executive Summary

The past two decades of national investments in computer science and high-performance computing have placed the DOE at the forefront of many areas of science and engineering. This initiative capitalizes on the significant gains in computational science and boldly positions the DOE to attack global challenges through modeling and simulation. The planned petascale computer systems and the potential for exascale systems shortly provide an unprecedented opportunity for science; one that will make it possible to use computation not only as a critical tool along with theory and experiment in understanding the behavior of the fundamental components of nature but also for fundamental discovery and exploration of the behavior of complex systems with billions of components including those involving humans.

Through modeling and simulation, the DOE is well-positioned to build on its demonstrated and widely-recognized leadership in understanding the fundamental components of nature to be a world-leader in understanding how to assemble these components to address the scientific, technical and societal issues associated with energy, ecology and security on a global scale.

In order to realize this leadership the DOE recognizes that the time-honored, or subsystems, approach in which the forces and the physical environments of a phenomenon are analyzed, is approaching a state of diminishing returns. The approach for the future must be systems based and simulation programs are developed in the context of encoding all known relevant physical laws with engineering practices, production, utilization, distribution and environmental factors.

This new approach will

- **Integrate, not reduce.** The full suite of physical, chemical, biological, chemical and engineering processes in the context of existing infrastructures and human behavior will be dynamically and realistically linked, rather than focusing on more detailed understanding of smaller and smaller components.
- **Leverage the interdisciplinary approach to computational sciences.** Current algorithms, approaches and levels of understanding may not be adequate. A key challenge in development of these models will be the creation of a

framework and semantics for model interaction that allow the interconnection of discipline models with observational data. At the outset, specialized scientific groups will team with engineers, business experts, ecologists and human behavior specialists comprehensive models, that incorporate all known phenomena and have the capability to simulate systems characteristics under the full range of uncertainties.

- **Capitalize on developments in data management and validation of ultra-large datasets.** It will develop new approaches to data management, visualization and analysis that can treat the scale and complexity of the data and provide the insight needed for validation of the computations.

This new approach will enable DOE to exploit recent developments in commercially available computer architectures, driven by the implementation of first generation multi-core processors and the introduction of petascale computers within 18 months, and prepare it to take advantage of exascale computers in the next decade. This approach will also guarantee DOE's leadership in applying these computers to critical problems confronting the nation.

The initiative has four programmatic themes:

1. **Engage** top scientists and engineers, computer scientists and applied mathematicians in the country to develop the science of complexity as well as new science driven computer architectures and algorithms that will

be energy efficient, extremely scalable, and tied to the needs of scientific computing at all scales. Correspondingly, recruit and develop the next generation of computational and mathematical scientists.

2. **Invest** in pioneering large-scale science, modeling and simulation that contribute to advancing energy, ecology and global security.
3. **Develop** scalable analysis algorithms, data systems and storage architectures needed to accelerate discovery from large-scale experiments and enable verification and validation of the results of the pioneering applications. Additionally, develop visualization and data management systems to manage the output of large-scale computational science runs and in new ways to integrate data analysis with modeling and simulation.
4. **Accelerate** the build-out and future development of the DOE open computing facilities to realize the large-scale systems-level science required to advance the energy, ecology and global security program. Develop an integrated network computing environment that couples these facilities to each other, to other large-scale national user facilities and to the emerging international network of high-performance computing systems and facilities.

The success of this fourth effort is built on the first three themes because exascale systems are, by themselves, among the most complex systems ever engineered.

This initiative will enable DOE to address critical challenges in areas such as:

Energy- Ensuring global sustainability requires reliable and affordable pathways to low-carbon energy production, e.g. bio-fuels, fusion and fission, and distribution on a massive scale. The existing mix of energy supplies places global security at great risk. Acceptable solutions require rapid and unprecedented scientific and technologic advances. Unfortunately, existing analytical, predictive, control, and design capabilities will not scale. An objective of this initiative is to provide new models and computational tools with the functionality needed to discover and develop complex processes inherent in a new energy economy.

Ecological Sustainability- The effort toward sustainability involves characterizing the conditions for balance in the climate system. In particular, sustainable futures involve understanding and managing the balance of chemicals in the atmosphere and ocean. The ability to fit energy production and industrial emissions within balanced global climate and chemical cycles is the major scientific and technical challenge for this century.

Security- The internet, as well as the instrumentation and control systems for the energy infrastructure, is central to the well-being of our society. There are several potential opportunities relating to accurately modeling these complex systems: understand operational data, identify anomalous behavior to isolate the disturbance and automatically repair any damage.

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